

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Dynamical matrix in magnetoelectrics¹ RAFFAELE RESTA, Physics Dept., Univ. of Trieste — In ordinary dielectrics the dynamical matrix at the zone center is a nonanalytic function of degree zero in the wavevector \mathbf{q} . Its expression (for a crystal of arbitrary symmetry) is well known and is routinely implemented in first principle calculations. The nonanalytic behavior occurs in polar crystals and owes to the coupling of the macroscopic electric field \mathbf{E} to the lattice. In magnetoelectric crystals both electric and magnetic fields, \mathbf{E} and \mathbf{H} , are coupled to the lattice, formally on equal footing. I provide the general expression for the zone center dynamical matrix in a magnetoelectric, where the \mathbf{E} and \mathbf{H} couplings are accounted for in a symmetric way. As in the ordinary case, the dynamical matrix is a nonanalytic function of degree zero in \mathbf{q} , and is exact in the harmonic approximation. Besides the above major result, I will also discuss other related issues: (i) The Lyddane-Sachs-Teller relationship for MEs, where the fields \mathbf{E} and \mathbf{H} are (once more) dealt with in a symmetric way; (ii) The microscopic origin of the coupling of magnetic fields to the lattice, which may look counter-intuitive; (iii) The relationship to first-principle implementations, where in the simplest cases \mathbf{E} and \mathbf{B} (not \mathbf{H}) are zero.

¹Partially supported by ONR Grant N00014-11-1-0145.

Raffaele Resta
Physics Dept., Univ. of Trieste

Date submitted: 28 Oct 2011

Electronic form version 1.4